The Linear Vector Space

We know that the state of a particle may be represented by a simple plane wave or by a combination of two or large number of plane waves (in the form of a wave packet) depending upon the form of the potential in which the particle is moving. The state (ψ) of the ~~partcle~~ particle is obtained by solving the corresponding Schrodinger equation of the particle. The Schrodinger equation is a linear equation and therefore the solutions (ie, the eigenstates of the particle) obey the principle of linear superposition. Therefore if ψ_1 and ψ_2 are the solutions of Schrodinger equation (ie are the ~~Ham~~ eigenstates of the Hamiltonian operator), the other solutions (ψ) can be constructed of the form

$$\psi = c_1\psi_1 + c_2\psi_2 \quad \text{—— (1)}$$

where c_1 and c_2 are arbitrary constants.

The situation seems to be analogous to the vectors in ordinary space, where any vector $\vec{R}$ may be expressed as a linear combination of unit vectors $\hat{e}_1, \hat{e}_2, \hat{e}_3$. It can be shown that the set of eigenstates $\{\psi_n\}$ of a Hermitian operator act in the so-called linear vector space at the same footing as unit vectors $\hat{e}_1, \hat{e}_2, \hat{e}_3$ do in the ordinary space.

Some characteristics of eigenstates of Hermitian operators

Let us consider the eigenstates of the energy operator of Hamitonian operator (Hamiltonian operator is a Hermitial operator because $H^{\dagger} = H$). While solving the Schrodinger equation of a particle in a simple one dimensional potential (like particle in a potential box), we found expressions of the set of allowed eigenstates. For example in case of a particle in potential box with rigid boundary conditions, we get the eigenstates as

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin \frac{n x \pi}{L} \quad \text{—— (2)}$$

These eigenstates have orthnormal properties expressed as

$$\int_0^L \psi_n^*(x)\,\psi_n(x)\,dx = 1 \quad \text{—— (3a)}$$

$$\int_0^L \psi_n^*(x)\,\psi_m(x)\,dx = 0 \quad \text{for } n \neq m \quad \text{—— (3b)}$$

For example let us see what will happen if we take a linear combination of all wave functions of the set $\{\psi_n\}$.

Let us call this sum as $f(x)$.

$$\therefore f(x) = \sum_n a_n \psi_n(x) \quad \text{—— (4a)}$$

$$= \sqrt{\frac{2}{L}} \sum a_n \sin \frac{n\pi x}{L} \quad ; \; n = 1, 2, 3 \cdots \quad \text{—— (4b)}$$

From the Fourier series analysis of functions, we see that that any function $f(x)$ within the interval $[0, L]$ satisfying the condition $f(x=0) = f(x=L) = 0$, may be expressed as a linear combination of functions $\sin\left(\frac{n\pi x}{L}\right)$ and therefore as a linear combination of eigenstates $\psi_n(x)$.

For a given function $f(x)$, we may find out the coefficients a_n as follows:

From eq^n. (4b) we get

$$\sqrt{\frac{2}{L}} \int_0^L f(x) \sin \left(\frac{m\pi x}{L}\right) dx$$

$$= \sum_n a_n \left[\left(\frac{2}{L}\right) \int_0^L \sin\left(\frac{n\pi x}{L}\right) \cdot \sin\left(\frac{m\pi x}{L}\right) dx \right]$$

$$= \sum_n a_n \delta_{mn}$$

$$= a_m$$

$\therefore$ So $$a_m = \sqrt{\frac{2}{L}} \int_0^L f(x) \sin\left(\frac{n\pi x}{L}\right) dx \quad \text{— (5a)}$$

or, $$\boxed{a_m = \int_0^L f(x)\, \psi_m(x)\, dx} \quad \text{— (5b)}$$

2nd Example

Consider a particle which is in a potential box with periodic boundary conditions. Suppose the potential box of width 2L, extending from $x=-L$ to $x=+L$.

The eigenstates are

$$\psi_n(x) = \frac{1}{\sqrt{2L}} e^{i\left(\frac{n\pi x}{L}\right)} \quad — (6)$$

The eigenstates have orthonormal properties expressed as

$$\int_{-L}^{L} \psi_n^*(x)\,\psi_n(x) = 1 \quad —— (7a)$$

and

$$\int_{-L}^{L} \psi_n^*(x)\,\psi_m(x) = 0 \text{ for } n \neq m \quad — (7b)$$

Let us take a linear combination of all wave functions and call this sum as $f(x)$

$$f(x) = \sum_n b_n \psi_n(x) \quad —— (8a)$$

$$\therefore f(x) = \frac{1}{\sqrt{2L}} \sum b_n e^{i(n\pi x/L)} \;;\; n = 0, \pm 1, \pm 2, \cdots \quad — (8b)$$

On multiplying bothsides of eq^n (8b) by $\frac{1}{\sqrt{2L}} e^{-i(m\pi x/L)}$ and integrating we get

$$\frac{1}{\sqrt{2L}} \int_{-L}^{L} f(x)\, e^{-i(m\pi x/L)}\, dx = \sum b_n \left[\frac{1}{2L} \int_{-L}^{L} e^{i\pi x(n-m)/L}\right] dx$$

$$= \sum b_n \delta_{mn} = b_m$$

$\therefore$ The coefficient b_n are given by

$$\boxed{b_n = \frac{1}{\sqrt{2L}} \int_{-L}^{L} f(x)\, e^{-i(n\pi x/L)}\, dx} \quad — (9)$$

Now we will write down all the above equation in Dirac notations and discuss their analogy with the expansion of vectors in ordinary space in terms of unit vectors $\hat{e}_1, \hat{e}_2, \hat{e}_3$.

Dirac Bra and Ket Notations

Let us start with the integral

$$\int_{-L}^{L} \psi_n^*(x)\,\psi_m(x)\,dx \quad \text{— (1)}$$

We try to write it in a compact notion say

$$\langle \psi_n | \psi_m \rangle \text{ — (2)} \quad \text{or } \langle n|m\rangle \text{ — (3)}$$

Let a wavefunction $\psi_n(x)$ be noted by ket $|\psi_n(x)\rangle$ or simply as $|n\rangle$ and the complex conjugate $\psi_m^*(x)$ be denoted as bra $\langle\psi_m(x)|$ or simply as $\langle n|$.
Then in Dirac braket notation we can write

$$\int \psi_n^*(x)\,\psi_m(x)\,dx = \langle \psi_n|\psi_m\rangle = \langle n|m\rangle.$$

If the wavefunctions are orthonormal ie $\int \psi_n^*(x)\psi_m(x)\,dx = \delta_{mn}$
then in Dirac bra, ket notation we can write this as

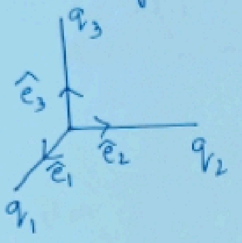
$$\langle \psi_n|\psi_m\rangle = \langle n|m\rangle = \delta_{mn} \text{ — (4)} \quad \left[\text{where } \delta_{mn} = 1 \text{ when } n=m,\ = 0 \text{ when } n \neq m\right]$$

ie, $\langle\psi_n|\psi_n\rangle = \langle\psi_m|\psi_m\rangle = 1 = \langle n|n\rangle = 1$ — (4a) and $\langle\psi_n|\psi_m\rangle = 0$ when $n \neq m$ $\therefore \langle n|m\rangle = 0$ — (4b)

and $$|f(x)\rangle = \sum_n b_n |\psi_n(x)\rangle = \sum_n b_n |n\rangle \quad \text{— (5)}$$

Let us now consider usual 3-D ordinary space expressed in Cartesian cordinate system. Let the three mutually perpendicular cordinate axes be denoted by q_1, q_2, q_3 and unit vectors along these three axes as $\hat{e}_1, \hat{e}_2, \hat{e}_3$.

These are also known as basis vectors in ordinary 3-D space.



$$\hat{e}_i \cdot \hat{e}_j = 0 \text{ when } i \neq j \quad \text{— (6a)}$$

$$\text{and } \hat{e}_i \cdot \hat{e}_i = 1 \quad (i = 1, 2, 3,\ j = 1, 2, 3) \quad \text{— (6b)}$$

Also any position vector $\vec{R}$ may be expressed as

$$\vec{R} = R_1 \hat{e}_1 + R_2 \hat{e}_2 + R_3 \hat{e}_3 = \sum_{i=1}^{3} R_i \hat{e}_i \quad \text{— (7)}$$

Thus if we compare the eqns (4a), (4b) and (5) with the eqns. given in eqns. (6a), (6b) and (7) we find similarities

(1) The three unit vector $\hat{e}_i$ are of unit length i.e their dot product $\hat{e}_i \cdot \hat{e}_i = 1$.

(2) The three unit vectors are normal to each other i.e, $\hat{e}_i \cdot \hat{e}_j = 0$ when $\hat{i} \neq \hat{j}$

(3) And any vector $\vec{R}$ can be expressed in terms of their linear combination i.e

$$\vec{R} = R_1 \hat{e}_1 + R_2 \hat{e}_2 + R_3 \hat{e}_3 = \sum_{i=1}^{3} R_i \hat{e}_i.$$

Similarly the eigenfunctions $\psi_n(x)$ or $(= |\psi_n\rangle = |n\rangle)$

① are normalized to unity ie $\langle\psi_n|\psi_n\rangle = \langle n|n\rangle = 1$

② are orthogonal to each other ie, $\langle\psi_n|\psi_m\rangle = \langle n|m\rangle = 0$ when $n \neq m$

③ are able to express any function $|f(x)\rangle$ in terms of their linear combination like $|f(x)\rangle = b_1\psi_1 + b_2\psi_2 + \cdots\cdots$

$$= \sum_{n=0}^{\infty} b_n|\psi_n\rangle = \sum_{n=0}^{\infty} b_n|n\rangle$$

Then it is evident that the set of eigenfunctions $|\psi_n\rangle = |n\rangle$ may be treated as basis (unit) vectors in the hypothetical finite or infinite space known as linear vector space or wave function space.

These basis vectors $|\psi_n\rangle = |n\rangle$ are having similar characteristics in linear vector space as ordinary unit basis vectors $(\hat{e}_i)$ have in ordinary space.

These unit or basis vectors $|n\rangle = |\psi_n\rangle$ are sometimes known as ket basis vectors in linear vector space (hypothetical space). The function $|f(x)\rangle$ formed out of linear combination of basis vectors $|\psi_n\rangle = |n\rangle$ is also a state vector in the linear vector space.

The linear vector space when complete is known as Hilbert space.

It may be mentioned here, explicitly that the mathematical definition of orthonormality of unit vectors in ordinary space and that of orthonormality of basis vectors (state vector $|\psi_n\rangle = |n\rangle$) in linear vector space are different. For example

$$\hat{e}_i \cdot \hat{e}_j = 0 \quad \text{and} \quad \hat{e}_i \cdot \hat{e}_i = 0 \quad \text{in ordinary space}$$

when $i \neq j$

and $\langle n|n\rangle = \int \psi_n^*(x)\, \psi_n(x)\, dx = 1$

and $\langle n|m\rangle = \int \psi_n^*(x)\, \psi_m(x)\, dx = 0, \quad n \neq m$ } in linear vector space

But these respective definitions of orthonormality lead to similar concept

(i) $\vec{R}$ can be expressed as a linear combination of unit vector $\hat{e}_i$ in ordinary space and a state vector $|u\rangle$ can be expressed as the linear combination of state unit vectors or basis vectors $|n_1\rangle, |n_2\rangle \ldots$ etc.

(ii) Dot product of two vectors $\vec{R} = \sum_{i=1}^{3} R_i \hat{e}_i$, $\vec{S} = \sum_{j=1}^{3} S_j \hat{e}_j$ is written as $\vec{R}\cdot\vec{S} = \sum_{i=1}^{3} R_i S_i = R_1 S_1 + R_2 S_2 + R_3 S_3$.

and the scalar product or inner product of two state vectors $|u\rangle$ and $|v\rangle$ in linear vector space is given by

When $f(x)$ ← $|u\rangle = \sum_n c_n |\psi_n\rangle = \sum_n c_n |n\rangle$

$|v\rangle = \sum_n d_n |\psi_n\rangle = \sum_n d_n |n\rangle$

$\therefore \langle u|v\rangle = \sum c_n^* d_n \langle n|n\rangle = \sum c_n^* d_n \Rightarrow$ complex no.

The eigenstates $|n\rangle$ of an operator $\hat{A}$ (say) form a complete set.

$$\langle m|u\rangle = \sum_n c_n \langle m|n\rangle = \sum_n c_n \delta_{mn} = c_m$$

We may write $|u\rangle = \sum |n\rangle c_n = \sum |n\rangle\langle n|u\rangle$

$$\boxed{\text{or, } \sum |n\rangle\langle n| = 1}$$

This is a <u>completeness condition</u>.